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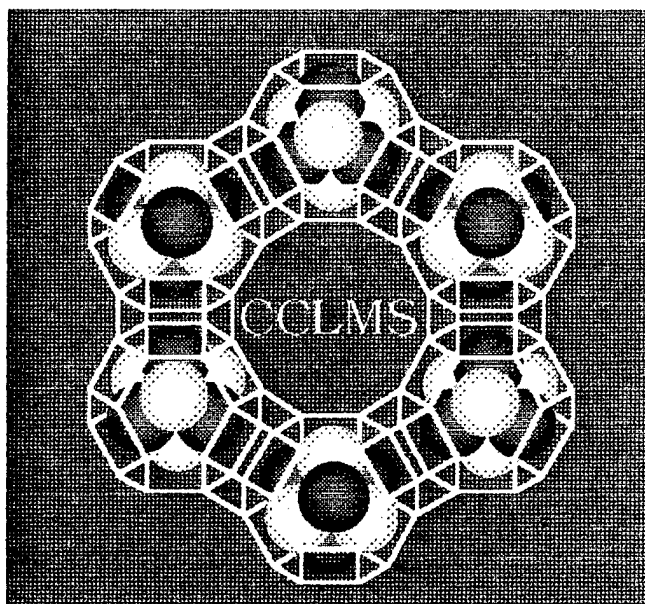
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STRUCTURE AND INTERFACE PROPERTIES OF NANOPHASE CERAMICS:
MULTIMILLION PARTICLE MOLECULAR-DYNAMICS SIMULATIONS ON
PARALLEL COMPUTERS

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DEPARTMENT OF PHYSICS AND ASTRONOMY
AND
DEPARTMENT OF COMPUTER SCIENCE
LOUISIANA STATE UNIVERSITY

FINAL TECHNICAL REPORT (1994-97)

PROPOSAL TITLE: Structure and Interface Properties of Nanophase Ceramics: Multimillion Particle Molecular-Dynamics Simulations on Parallel Computers

GRANT NUMBER: F49620-94-1-0444

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EXECUTIVE SUMMARY

Large-scale molecular-dynamics (MD) simulations were performed to investigate: i) sintering process, structural correlations, and mechanical behavior including dynamic fracture in microporous and nanophase Si_3N_4 ; ii) crack-front propagation in amorphous silica; iii) hypervelocity impact damage in diamond films and crack-front instabilities in graphite; iv) phonons in graphitic tubules; and v) amorphization and fracture in nanowires. The simulations were carried out with highly efficient multiscale algorithms and dynamic load-balancing schemes for mapping irregular atomistic simulations on distributed-memory parallel architectures. These research activities resulted in twenty-four journal publications and thirty invited presentations. Two graduate students received dual-degrees--Ph.D. in physics and a M.S. from the Department of Computer Science--during the course of this project.

This project involved two faculty members, two graduate students, and a postdoc. It also involved interactions/transitions with researchers at governmental laboratories and industry.

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§ 1 BACKGROUND

Advanced ceramics are excellent materials for applications requiring extreme operating conditions. The capability to withstand high temperatures, combined with their high strength and low weight, makes them highly desirable for aerospace applications such as high thrust-to-weight ratio turbine engines, hypersonic aerospace vehicles, and space satellites. These materials are also very useful for surface transportation, electronics, and advanced manufacturing industries.

The fundamental issue concerning ceramics is the relationship between the microscopic structure, atomic diffusion, and mechanical and thermal properties. An understanding of this relationship on the atomic scale is critical for the design of novel ceramics with application-specific properties.

This DEPSCoR project involved the investigation of properties and processes in nanostructured ceramics. Using large scale molecular-dynamics (MD) simulations, we investigated:

- Structural correlations and mechanical behavior, including crack-front propagation, in crystalline and nanophase silicon nitride;
- Growth of pore interfaces and brittle and ductile behavior in amorphous silica;
- Mechanical properties, thermal transport, and low-frequency floppy modes in microporous silicon nitride;
- Early stages of sintering of ceramic nanoclusters;
- Damage in diamond coatings due to particle impact;
- Crack propagation in graphite;
- Strain effects and phonons in graphitic tubules;
- Amorphization and fracture in nanowires.

These MD simulations were executed with highly efficient, portable and scalable, multiresolution algorithms including the fast multipole method for the long-range Coulomb interaction and a dynamic load-balancing scheme for mapping irregular applications on parallel machines. *These research activities have resulted in 24 journal papers and 30 invited presentations.* The next section provides an overview of our research accomplishments.

§ 2 RESEARCH ACCOMPLISHMENTS

§ 2.1 STRUCTURE AND MECHANICAL PROPERTIES OF NANOPHASE Si_3N_4

Advanced ceramics such as Si_3N_4 , SiC , SiO_2 , and Al_2O_3 are highly desirable materials for applications requiring extreme operating conditions. Light weight, elevated melting temperatures, high strengths, and wear and corrosion resistance make them very attractive for applications in aeronautics, automotive, electronics, and advanced manufacturing industries. The only serious drawback of ceramics is that they are brittle at low to moderately high temperatures.

In recent years a great deal of progress has been made in the synthesis of ceramics that are much more ductile than conventional coarse-grained materials. (These so called nanophase materials are fabricated by in-situ consolidation of nanometer size clusters.) Despite a great deal of research, many perplexing questions concerning nanophase ceramics remain unanswered. Experiments have yet to provide information regarding the morphology of pores or the structure and dynamics of atoms in nanophase ceramics. As far as modeling is concerned, only a few

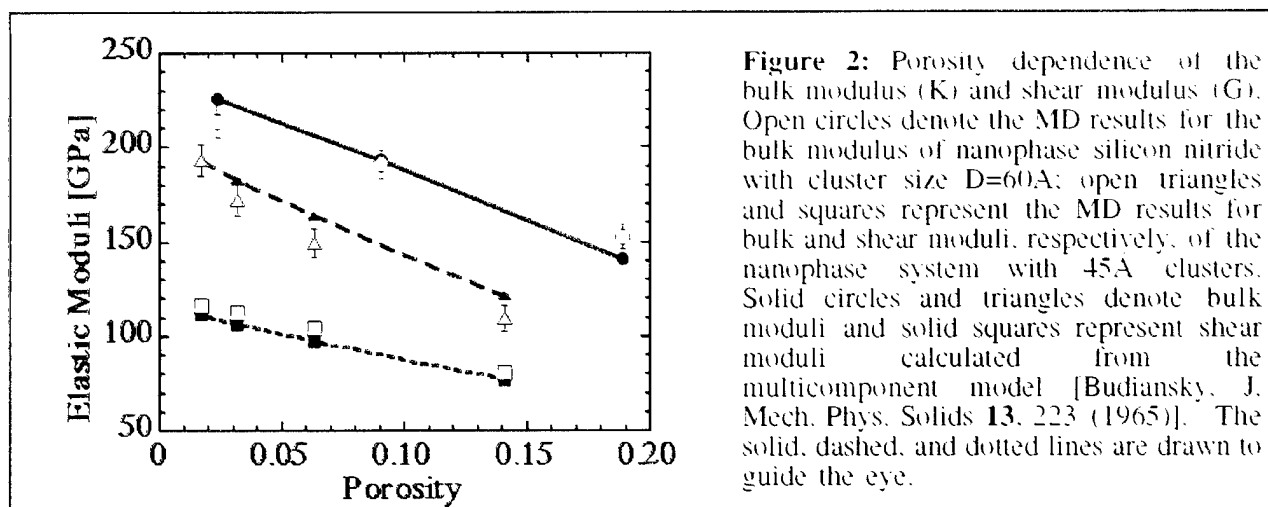
atomistic simulations of nanophase materials have been reported thus far. (This is due to the fact that these simulations are computationally very demanding: A realistic simulation of a nanophase solid requires 10^5 - 10^6 time steps for processing and $\sim 10^6$ atoms, since each nanocluster itself consists of 10^3 - 10^4 atoms.)

Using 1.08 million particle MD simulations we have investigated the structure and mechanical behavior of nanophase Si_3N_4 . The MD simulations are performed with effective two- and three-body interatomic potentials: The two-body terms consist of steric repulsion between atoms, screened Coulomb potentials due to charge transfer between Si and N, and a charge-dipole interaction that takes into account the large electronic polarizability of nitrogen; the three-body potential in Si_3N_4 takes into account covalent effects through bond-bending and bond-stretching terms. To establish the validity of this interaction scheme, we compare the MD results with a variety of experimental measurements. We find: i) the bond lengths and bond-angle distributions in crystalline and amorphous Si_3N_4 are in excellent agreement with experiments; ii) the positions and relative heights of the peaks in the static structure factor for amorphous Si_3N_4 are in good agreement with neutron scattering measurements; iii) the phonon density-of-states of crystalline α - Si_3N_4 agrees well with inelastic neutron scattering experiments; iv) the specific heat of crystalline α - Si_3N_4 is in excellent agreement with experiments over a wide range of temperatures; and v) the bulk modulus and Young's moduli along different directions in α - Si_3N_4 deviate less than 10% from the experimental values.



Figure 1: Snapshot of a configuration of nanophase Si_3N_4 before consolidation (left). The other picture shows the system consolidated with an applied pressure of 15 GPa. The density of the consolidated system is 2.94 g/cc which is 92% of the density of the α - Si_3N_4 crystal.

Nanophase Si_3N_4 is generated by consolidating a random cluster configuration (108 clusters with 10,052 atoms each) with the constant-pressure MD approach. Figure 1 shows the nanophase systems before and after consolidation under an applied pressure of 15 GPa. Pair-distribution functions and bond-angle distributions reveal that interfacial regions in the consolidated nanophase Si_3N_4 are amorphous and they contain a large number of undercoordinated Si atoms. Systems sintered at low pressures (~ 1 GPa) have percolating pores whose surface roughness exponents (0.46 and 0.86) are in excellent agreement with experiments. We also find that the dependence of elastic moduli on porosity and grain size in nanophase Si_3N_4 can be understood in terms of a three-phase model for heterogeneous materials (please see Fig. 2).



§2.2 CRACK-FRONT PROPAGATION IN NANOPHASE SILICON NITRIDE

Understanding the role of microstructures in fracture is one of the most challenging problems in materials science. Nanophase materials are ideal systems to examine this issue at the atomistic level since microstructures in these materials are only a few nanometers in dimension. Using 1.08 million particle MD simulations, we have investigated the morphological and dynamic aspects of fracture in nanophase Si_3N_4 . Figure 3 shows snapshots of the crack front at various values of the external strain. The crack front consists of pores connected to the notch (shown in magenta; the remaining disconnected pores are shown in orange). Figure 3 (a) shows a snapshot taken 10 ps after the notch is inserted. We observe initial development of the crack front and the growth of a few crack branches in the system. These local branches and nanoclusters tend to arrest the motion of the crack front, and further crack propagation is only possible if additional strain is applied. Figure 3(b) shows a snapshot of the crack front in the nanophase system under 11% strain. Comparing with Fig. 3(a), it is evident that the crack front has advanced significantly and coalesced with the pores in the center. We also observe that pores and interfacial regions allow the crack front to meander and form a branched structure. Figure 3(c) shows a crack-front snapshot 10 ps after the system was strained to 14%. At this time a secondary crack (top left hand corner of the figure) with several local branches merges with the primary crack. With further increase in the strain the secondary front advances toward the initial notch while the crack keeps growing laterally. When the strain reaches 30%, the crack finally separates the material into two disconnected parts and the system is now completely fractured. It should be noted that the critical strain (30%) at which the nanophase system fractures is enormous compared to what the crystalline Si_3N_4 system can sustain (at an applied strain of only 3% the crystal undergoes cleavage fracture). This is due to: i) plastic deformation in interfacial regions; ii) deflection and arrest of cracks by nanoclusters; and iii) multiple crack branching. None of these mechanisms are operative in the crystalline system. This demonstrates the dramatic effect of nanostructures on fracture.

To compare the toughness of nanophase and crystalline systems, we have calculated the fracture energy per unit area in both nanophase and crystalline Si_3N_4 systems (with the same geometry). For the (10 $\bar{1}$ 0) surface of an atomically sharp mode I crack (film surface was (0001)) in an α - Si_3N_4 crystalline film, the stress distribution was calculated using the MD method. From the prefactor of the $r^{-0.5}$ term of the local stress (r is the distance from the crack tip), we have estimated the critical stress-intensity factor. This analysis gives a value which is close to our MD

estimate of the intrinsic toughness ($1.3 \text{ MPa}\cdot\text{m}^{0.5}$). From the calculations of the fracture energy per unit area, we estimate that the toughness of the nanophase Si_3N_4 is six times larger than that of the crystal.

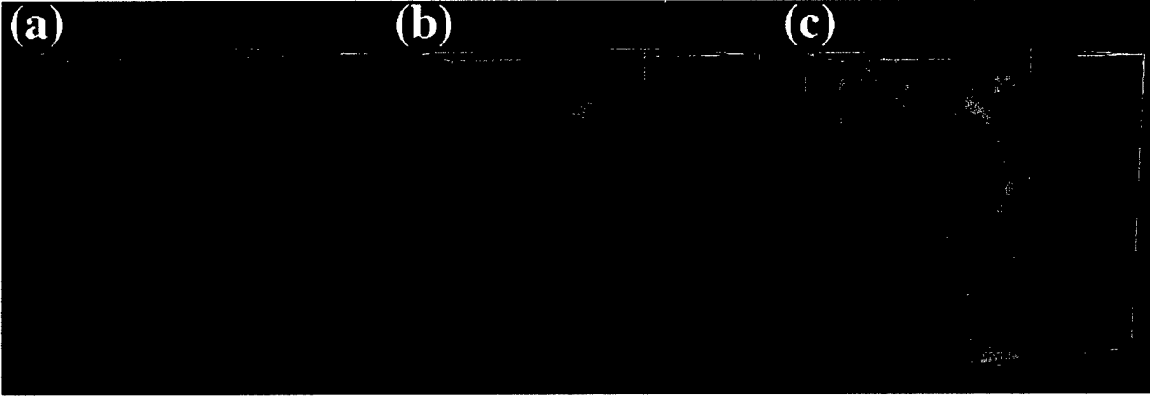


Figure 3: Snapshots of the crack front (shown in magenta) along with large ($>6.4 \text{ nm}^3$) isolated pores (shown in orange) in the strained nanophase system: a) Initial notch with crack branches and pores in the system under an applied strain of 5%; b) the primary crack front after the strain is increased to 11%; and c) the primary and secondary crack fronts at 14% strain on the system.

We have also investigated the morphology of crack fronts in the fractured nanophase Si_3N_4 . In recent years this issue has drawn a great of experimental attention. Measurements on a variety of brittle and ductile solids have revealed that the widths of fracture profiles scale with the lengths as $w \sim L^\zeta$. For out-of-plane fracture profiles, the roughness exponent, ζ_\perp , above a certain length scale, has a value of 0.8 in three and 0.7 in two spatial dimensions. Many experiments indicate that these values of ζ_\perp may be independent of the material or the mode of fracture. At small length scales or when the crack front propagates quasi statically, the roughness exponent crosses over to a smaller value ~ 0.5 . Recently it has also been pointed out that there is another distinct roughness exponent, $\zeta \approx 0.6$, associated with in-plane fracture profiles.

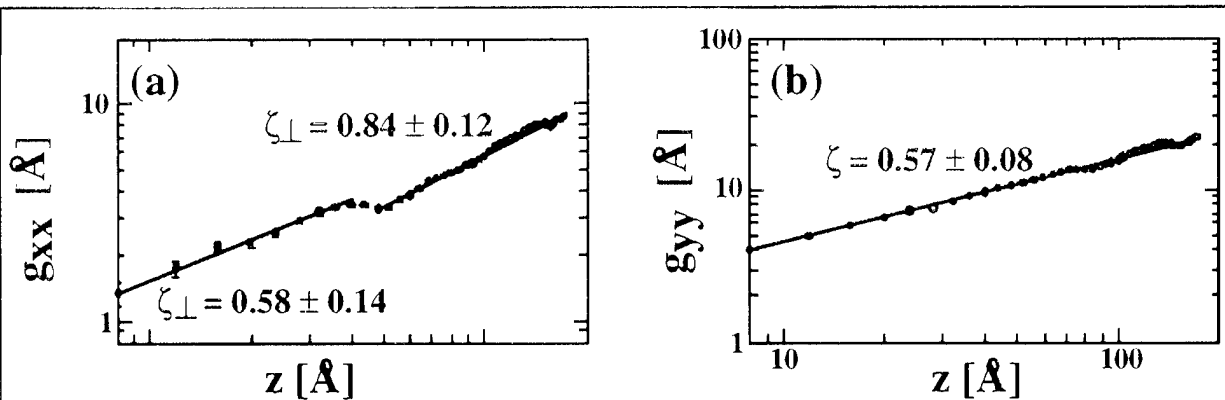
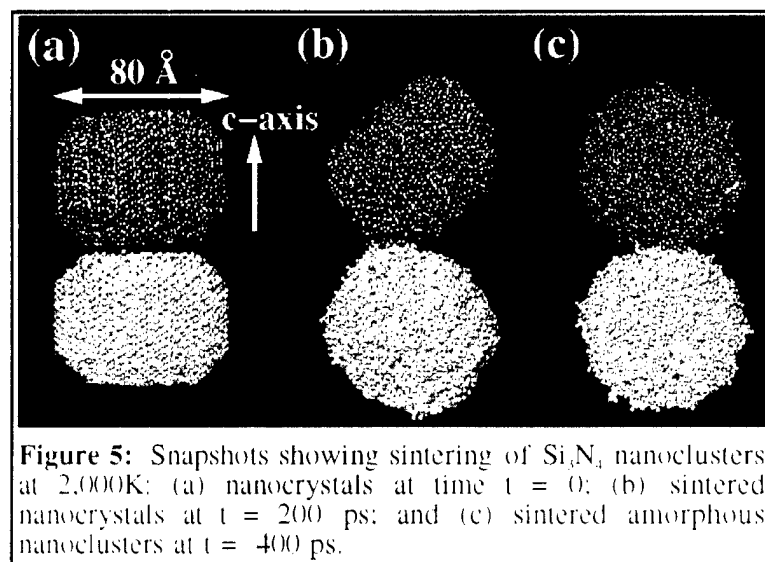


Figure 4: (a) log-log plot of the height-height correlation function, $g_{xx}(z)$, versus z for the out-of-plane fracture profile $x(z)$; (b) the variation of $g_{yy}(z)$ for the in-plane fracture profile $y(z)$.

To investigate the nature of self-affine fracture surfaces in nanophase Si_3N_4 , we calculate the height-height correlation functions both in and out of the fracture plane y - z . Figure 4a shows that the best fit to the out-of-plane height-height correlation function $g_{xx}(z)$ ($= \langle [x(z+z_0) - x(z_0)]^2 \rangle^{1/2}$) for the fracture profile $x(z)$ requires two roughness exponents: $\zeta_\perp = 0.84 \pm 0.12$ above a certain

length scale (64\AA) and $\zeta_{\perp} = 0.58 \pm 0.14$ otherwise. For the other out-of-plane height-height correlation function $g_{xx}(y)$, the roughness exponent $\zeta_{\parallel} = 0.75 \pm 0.08$. The MD results for ζ_{\perp} and ζ_{\parallel} are very close to experimental values. We have also determined the roughness exponent, ζ , for the in-plane fracture profile $y(z)$: Figure 4b shows that the best fit to the corresponding height-height correlation function gives $\zeta = 0.57 \pm 0.08$. Measurements of ζ in Al-Li and Supera α_2 Ti $_3$ Al-based alloys yield 0.60 ± 0.04 and 0.54 ± 0.03 , respectively [E. Bouchaud, J. Phys. Cond. Matter].

§ 2.3 SINTERING OF SILICON NITRIDE NANOCLUSTERS



The study of structural and mechanical properties of nanophase Si $_3$ N $_4$ was preceded by MD simulations of sintering of silicon nitride nanoclusters (each cluster consisting of 20,335 atoms). Our MD calculations provide a microscopic view of neck formation during early stages of sintering (Fig. 5). In the case of Si $_3$ N $_4$ nanocrystals at 2000K, we initially observe considerable relative motion of clusters. Subsequently a few Si and N atoms join the two nanocrystals and, thus bound, they continue to rotate relative to each

other for 100 ps. In the next 100 ps, the relative motion subsides and we observe a steady growth of an asymmetric neck between the two nanocrystals. In the neck region, there are more four-fold than three-fold coordinated Si atoms. We have also investigated the sintering of amorphous silicon nitride nanoclusters at 2,000K. The neck between amorphous nanoclusters is much more symmetric than the neck between thermally rough nanocrystals. The neck region between amorphous nanoclusters has nearly the same number of three- and four-fold coordinated Si atoms. For both nanocrystals and amorphous nanoclusters, sintering is driven by diffusion of surface atoms. The diffusion in the neck region of amorphous clusters is four times faster than in the neck between nanocrystals.

§ 2.4 FLOPPY MODES AND THERMAL TRANSPORT IN MICROPOROUS Si $_3$ N $_4$

Physical properties of Si $_3$ N $_4$ are greatly influenced by voids. (They are usually present in the system as a result of synthesis by chemical vapor deposition or other processes.) Using MD simulations we have investigated the effect of porosity on mechanical properties and thermal conductivity of amorphous Si $_3$ N $_4$. Under uniform dilation, pores begin to form at a mass density of $\rho = 2.6$ g/cc. With further decrease in the density, the number of pores and their sizes increase dramatically and around 2.0 g/cc the largest pore percolates through the system. Near percolation the average pore volume diverges as $(\rho - \rho_c)^{-\gamma}$ with $\gamma = 1.95 \pm 0.17$. This is consistent with the percolation theory.

The thermal conductivity of microporous Si $_3$ N $_4$ is calculated from the heat current-current correlation function and a non-equilibrium MD approach. Between 300 and 1500K, the thermal conductivity scales as ρ^t where $t \approx 1.5$. Experimental data on carbon and silica aerogels are in

agreement with this result. The MD results for Young's modulus E vary as ρ^τ with $\tau \approx 3.6$. This is also close to the experimental value of τ for silica aerogels.

The nature of low-energy floppy modes in microporous Si_3N_4 has also been investigated with the MD approach. Floppy modes appear continuously in amorphous Si_3N_4 as the network connectivity is reduced; in the crystal they appear suddenly at 20% volume expansion. We find that their contribution to density-of-states varies linearly with energy and they significantly enhance the specific heat of microporous Si_3N_4 .

§ 2.5 HYPERVELOCITY IMPACT DAMAGE IN A DIAMOND COATING

Recently researchers at Phillips Lab's Space Environment Interaction Branch have designed an experimental technique to simulate debris impact in low earth orbit (LEO) using micro-flyer plates. The latter simulate debris particles traveling at speeds in the range of 8-10 km/s. The plates are propelled by a laser beam inside a space chamber. Currently the debris experiments are performed with an expensive 60-foot-long gun.

In an attempt to simulate such debris-impact experiments on parallel computers, we have performed large-scale MD calculations to determine the hypervelocity impact damage caused by a diamond crystallite on a diamond coating. (Rocketdyne in collaboration with Phillips Laboratory are using chemical vapor deposition to apply thin films of diamond to surfaces for a wide range of rocket applications.) The MD simulations are based on a reactive bond order (REBO) potential proposed by Brenner [Phys. Rev. B **42**, 9458 (1990)]. This potential is quite unique in that it treats covalent bonding in molecular and solid-state structures with a single classical expression. Moreover, the potential can describe chemical processes such as covalent bond formation and breaking. The parameters of the potential have been fitted to experimental values and first-principles calculations of bond lengths, bond energies, and force constants for several solid-state and molecular systems. The REBO potential has been shown to provide a good description of various properties outside the fitting database such as elastic constants and vibrational spectra of diamond and in-plane elastic properties of graphite. The results for the surface reconstruction and energetics of point defects in diamond are also in good agreement with experiments and electronic-structure calculations. The calculated formation energies for an extensive set of hydrocarbon molecules agree well with experimental results.

We have performed three hypervelocity impact-damage simulations. In the first case the crystallite strikes the diamond film with a velocity of 8 km/s. The crystallite penetrates the film to a depth of 20 Å, causing the diamond structure of the film to graphitize without any crater formation. Subsequently the nearly-intact crystallite emerges from the coating at a speed of 4 km/s. In the second simulation the incoming crystallite strikes the coating at a speed of 11 km/s. Part of the crystallite disintegrates after impact, and almost all of its kinetic energy is imparted to the coating. In this case we observe the formation of a crater along with amorphization in the impact region. In the third case the crystallite hits the diamond coating at a velocity of 15 km/s. Unlike the first two cases, the crystallite completely disintegrates causing extensive damage including the creation of a crater.

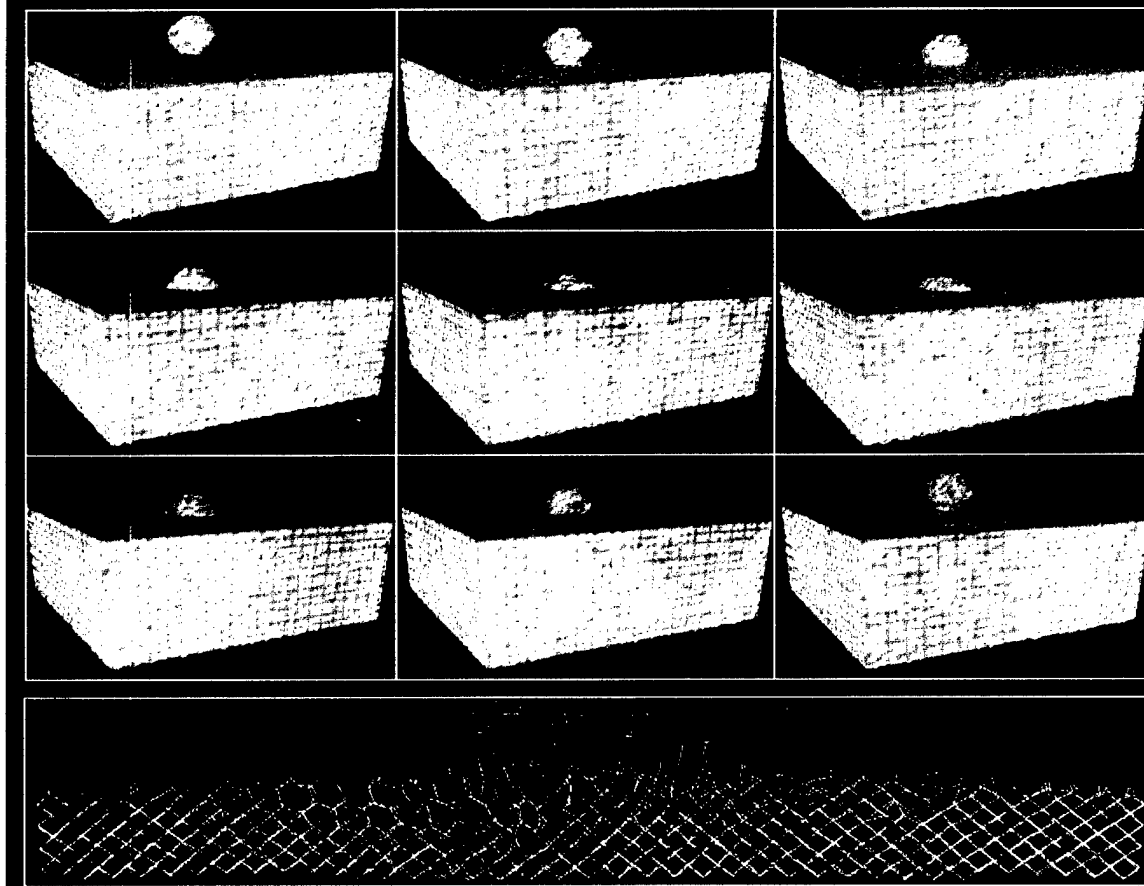


Figure 6: The first nine snapshots show the impact of a diamond crystallite on a diamond coating. These are the results of our million atom MD simulations over a time period of 28 pico seconds. The crystallite hits the coating at a speed of 8 km/s. After impact, it penetrates the coating and then bounces out at a speed of 4 km/s. The last snapshot shows that the energy imparted to the coating causes graphitization under the contact region.

§2.6 DYNAMIC FRACTURE IN A GRAPHITE SHEET

Recently we have also investigated crack propagation in a graphite sheet using million-atom MD simulations on parallel machines. (These simulations are also based on the reactive bond order potential of Brenner.) Fracture dynamics is investigated under a constant applied strain after inserting a notch of length 20\AA . We consider two different orientations of the graphite sheet, which exhibit completely different behavior during crack-front propagation:

- Under an applied uniaxial strain of 12% the system G(1,1), in which a fraction of covalent bonds are parallel to the strain (Fig. 7b), undergoes cleavage-like fracture;
- For the G(1,0) orientation, the crack front develops multiple secondary branches and overhangs (Fig. 7a) when its speed reaches approximately half the Rayleigh wave speed. Within the same secondary branch the crack-front profile has a roughness exponent $\zeta = 0.5$, whereas for interbranch fracture surface profiles $\zeta = 0.7$. The scenario of multiple local branches and the values of the roughness exponents are in agreement with recent experimental investigations of fracture.

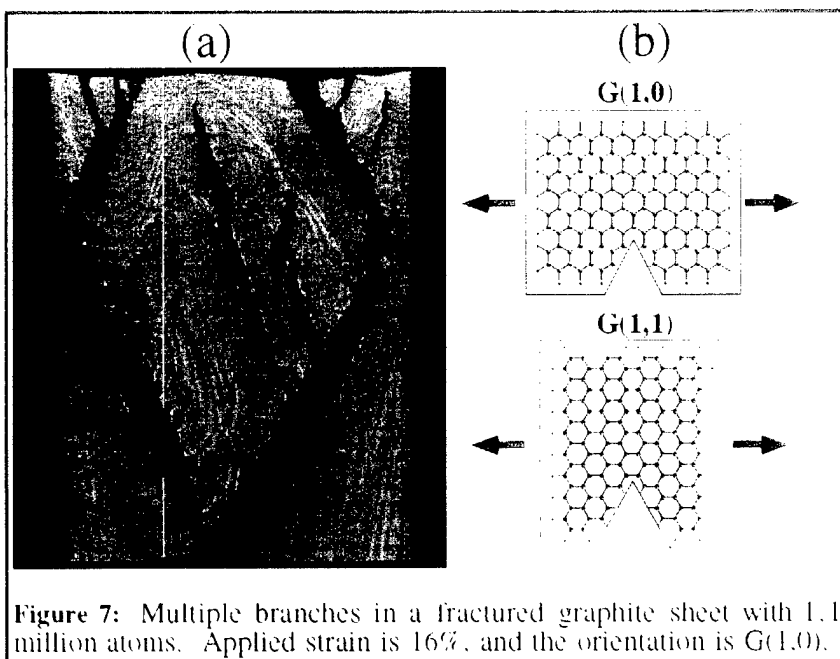


Figure 7: Multiple branches in a fractured graphite sheet with 1.1 million atoms. Applied strain is 16%, and the orientation is G(1,0).

as $\sigma_F \sqrt{c}$, where σ_F is the critical stress at which the crack starts propagating and c is the length of the notch) is found to be $4.7 \text{ MPa}\cdot\text{m}^{1/2}$. We have also calculated the local-stress distribution around the notch just before the onset of crack propagation. The data are well-described by $1/\sqrt{r}$ dependence with a stress-intensity factor of $6 \text{ MPa}\cdot\text{m}^{1/2}$. The angular dependence of the local stresses is also in good agreement with the elasticity theory.

§ 2.7 AMORPHIZATION AND FRACTURE IN NANOWIRES

Silicon diselenide is an important chalcogenide material. It is one of the basic solid electrolytes for advanced high-energy electrochemical cells. Recently we investigated the dynamics of amorphization and fracture in SiSe_2 nanowires using large-scale MD simulations. The calculations are based on interatomic potentials which combine charge-transfer, electronic polarizabilities, steric effects, and three-body covalent interactions. The validity of the interaction scheme is established by comparing the MD results with various available measurements. We find: structural correlations in both crystalline and amorphous systems are in excellent agreement with experiments; the calculated melting temperature ($1250 \pm 20 \text{ K}$) is very close to the experimental value ($1233 \pm 5 \text{ K}$); and the vibrational spectra of crystalline and amorphous SiSe_2 are also in good agreement with neutron scattering measurements.

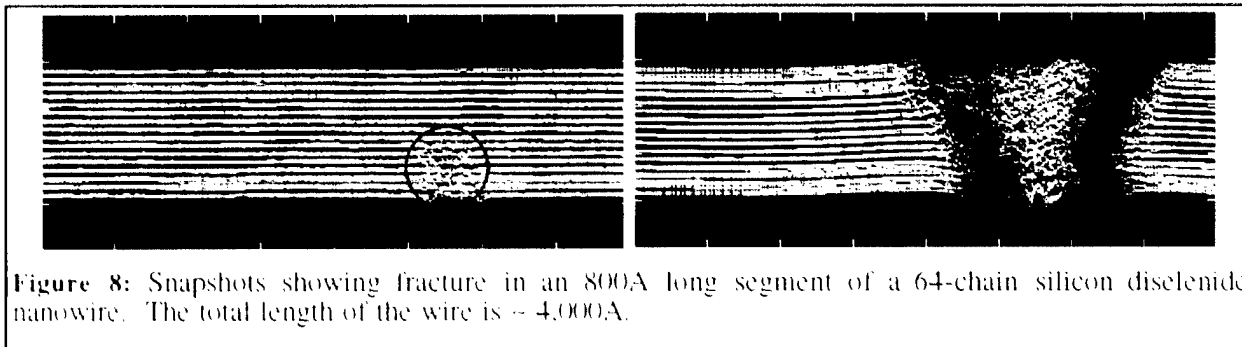


Figure 8: Snapshots showing fracture in an 800Å long segment of a 64-chain silicon diselenide nanowire. The total length of the wire is $\sim 4,000 \text{ Å}$.

The MD simulations for SiSe_2 nanowires reveal that the critical strain ($\sim 15\%$) of fracture is independent of the number of chains in the nanowire. Also fracture is preceded by amorphization

in nanowires. At first, bonds between edge-sharing tetrahedra break in the chains at the outermost layer. These broken chains form corner-sharing tetrahedra by cross-linking with neighboring chains. Local amorphization propagates across the nanowire to form a sandwich-like structure with an amorphous region in the middle. Cracks then nucleate at the boundaries and propagate inward from the nanowire surface until the nanowire fractures (Fig. 8).

§2.8 STRUCTURAL CORRELATIONS AND BRITTLE/DUCTILE BEHAVIOR IN AMORPHOUS SILICA

Silica has numerous technological applications in microelectronic devices and micro-electro-mechanical systems (MEMS). Atomistic simulations have been used to study the behavior of silica. We have investigated the fracture process in vitreous SiO_2 by applying the parallel multiresolution MD approach to a system of 1.18 million atoms. The calculations are based on an interatomic potential which includes the effects of charge transfer, electronic polarizabilities, and steric repulsion through two-body terms; covalent effects are included via three-body bond-bending and bond-stretching terms. Figure 9 shows a comparison between the MD and neutron-scattering results for the static structure factor, $S(q)$, of amorphous silica. Clearly the simulation results for $S(q)$ are in very good agreement with experiments. The calculations for elastic moduli and the phonon density-of-states of amorphous SiO_2 are also in good agreement with experimental measurements.

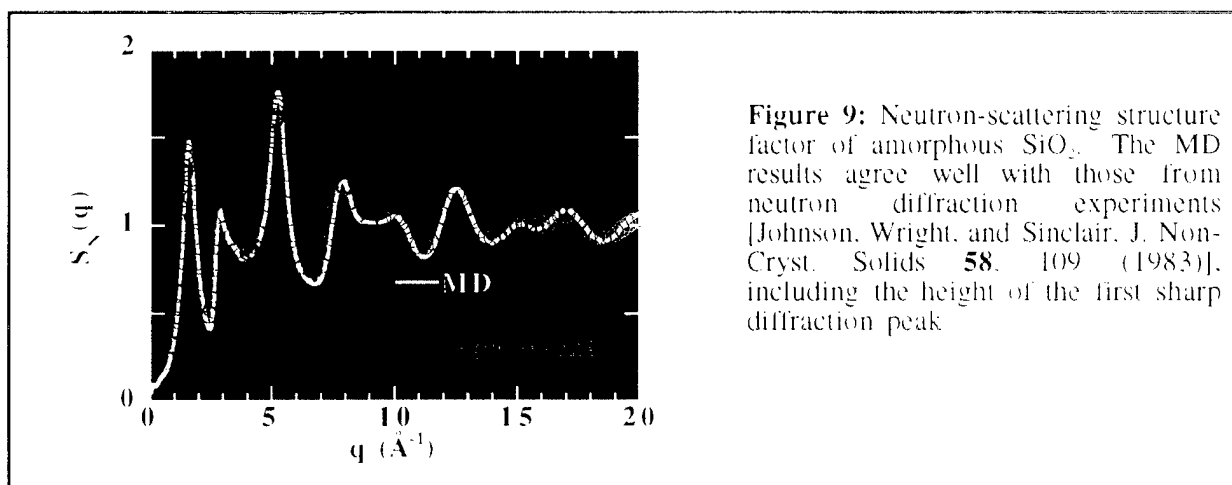
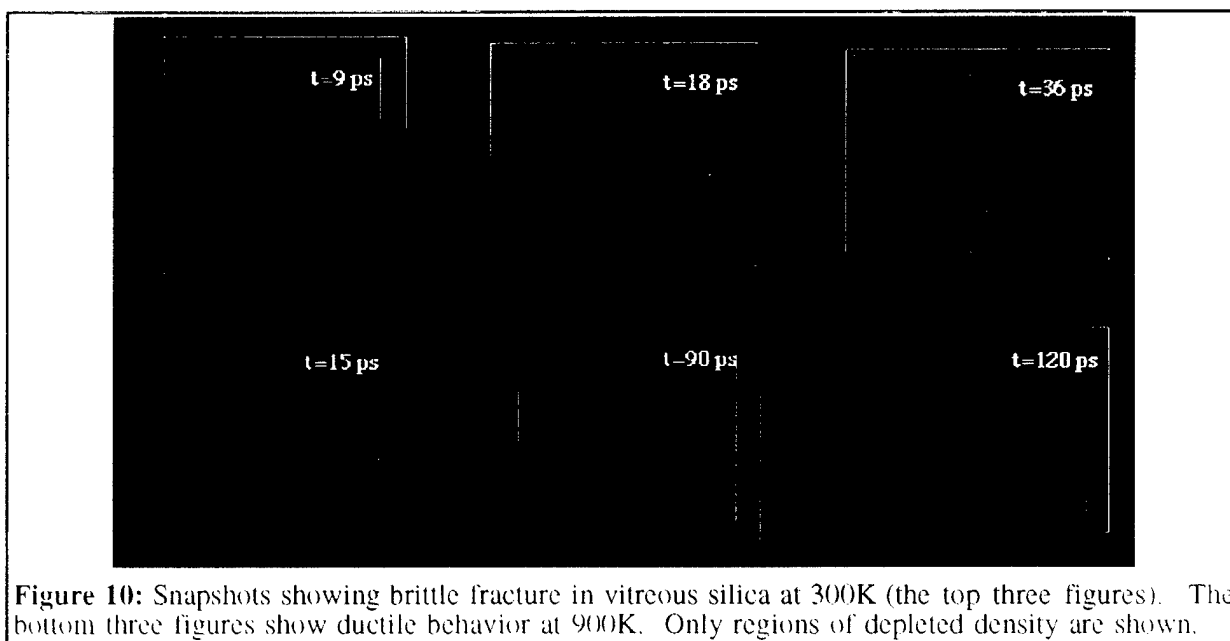


Figure 9: Neutron-scattering structure factor of amorphous SiO_2 . The MD results agree well with those from neutron diffraction experiments [Johnson, Wright, and Sinclair, *J. Non-Cryst. Solids* **58**, 109 (1983)], including the height of the first sharp diffraction peak.

Figure 10 shows the MD results for fracture (snapshots of crack fronts) in amorphous silica at 300K and 900K. It is evident that the system undergoes cleavage fracture at 300K. At the critical strain for fracture (8%), the crack tip reaches a terminal speed of 1.40 km/s which is nearly half the Rayleigh wave speed. (At 600K, the fracture is again cleavage-like with the terminal crack-tip speed reaching a value of 0.85 km/s.) In contrast, at 900K the amorphous silica system shows plastic behavior up to a strain of 17%. Currently we are investigating sintering, structural correlations, and mechanical properties of nanophase amorphous silica system.



§ 2.9 ATOMISTIC PROCESSES IN SILICON CARBIDE AND ALUMINA

Silicon carbide and alumina are excellent structural ceramics for applications requiring extreme operating conditions. We are investigating properties and processes in these materials using large-scale MD simulations. The SiC simulations are based on an empirical bond-order potential proposed by Tersoff [Phys. Rev. B **39**, 5566 (1989)]. The MD results for structural properties (bond lengths, bond angles, etc.), elastic moduli, and the cohesive energy of crystalline SiC are in excellent agreement with experiments. The melting temperature obtained from MD simulations using Tersoff's potential agrees well with the result of the electronic-structure calculations. Currently we are performing MD simulations to understand the crack-front morphology and the effect of strain rate on dynamic fracture in crystalline and amorphous SiC systems. Preliminary results of these fracture simulations are shown in Fig. 11.

The MD simulations for aluminum oxide are based on an interaction scheme proposed by Streitz and Mintmire [Phys. Rev. B **50**, 11996 (1994)]. This potential allows the local atomic charges to vary with the environment. The dynamic charge transfer and the resulting electrostatic interaction is merged with an embedded-atom potential yielding a scheme which can simultaneously treat FCC aluminum and α -alumina systems. This potential has been optimized to reproduce the bulk structural and mechanical properties of FCC aluminum and α -alumina. Additionally, the potential yields reasonable values for surface energies and surface relaxations.

We have implemented the MD simulations for Al_2O_3 using an extended Lagrangian scheme in which the charges are treated as dynamical variables. The long-range Coulomb interaction is implemented with an $O(N)$ fast multipole method (FMM). We have already determined the phonon density-of-states (DOS), infrared spectrum, and Raman spectrum of α - Al_2O_3 crystal. The MD results compare well with experimental measurements. Currently, we are investigating the behavior of $\text{Al}/\text{Al}_2\text{O}_3$ interface. The preliminary results are shown in Fig. 11.

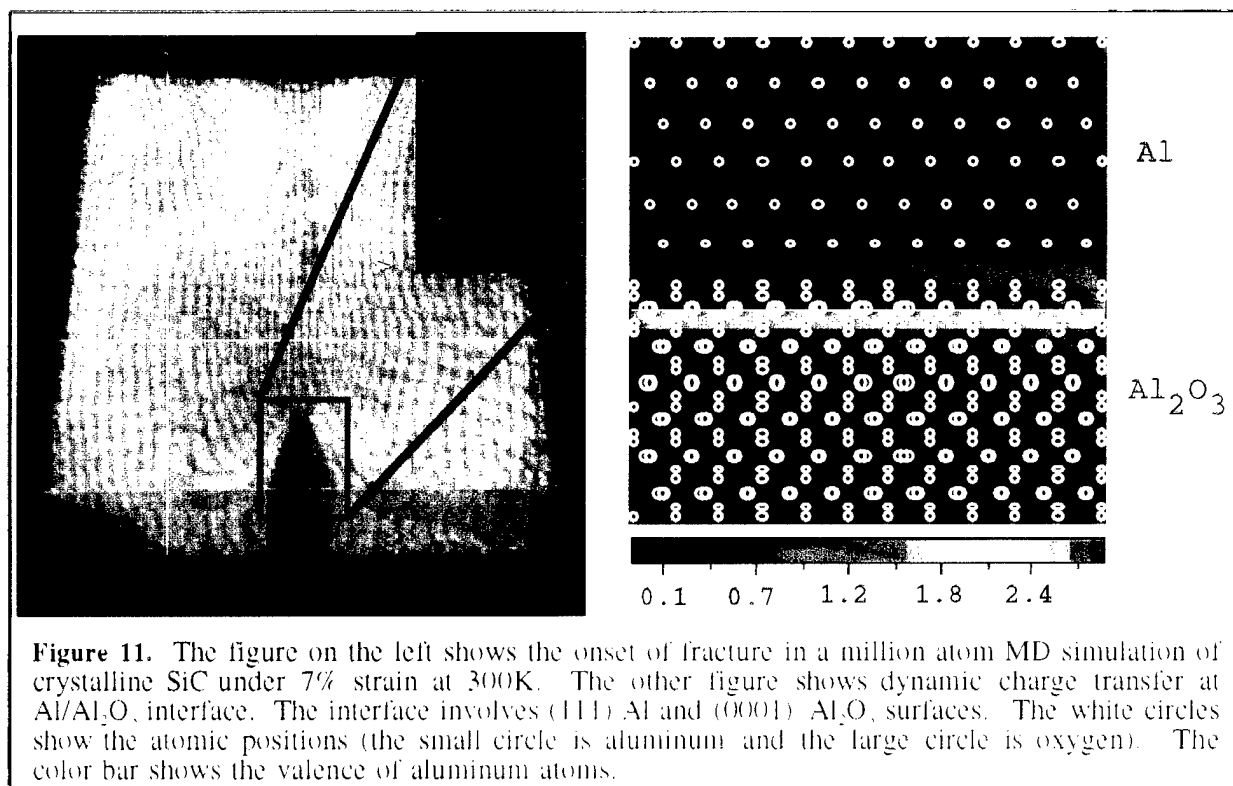


Figure 11. The figure on the left shows the onset of fracture in a million atom MD simulation of crystalline SiC under 7% strain at 300K. The other figure shows dynamic charge transfer at Al/Al₂O₃ interface. The interface involves (111) Al and (0001) Al₂O₃ surfaces. The white circles show the atomic positions (the small circle is aluminum and the large circle is oxygen). The color bar shows the valence of aluminum atoms.

§2.10 PARALLEL MULTIREOLUTION MOLECULAR-DYNAMICS SIMULATIONS

Atomistic simulations discussed in §2.1 - §2.9 require considerable computational resources because of long processing times, large systems, and compute-intensive interatomic interactions (e.g. long-range Coulomb and three-body covalent forces). These simulations are not feasible without efficient algorithms or massively parallel machines.

We have designed a highly efficient, multiresolution molecular-dynamics (MRMD) approach to carry out large-scale materials simulations on parallel machines. This approach includes the fast multipole method (FMM)--a divide-and-conquer scheme which reduces the computational cost for the Coulomb interaction from $O(N^2)$ to $O(N)$. The FMM is based on a hierarchical subdivision of space (Fig. 12), where at each spatial scale the influence of a large collection of charges is approximated to any desired precision by a multipole expansion. The method is well-suited to parallel architectures: Unlike the direct method which must communicate the locations and strengths of a large number of charges between distant processors, the FMM transmits a compressed representation of this information, namely the coefficients of the multipole expansion. In addition to FMM, the MRMD approach includes a multiple time-scale algorithm for short-ranged, two-body interactions and a separable scheme for three-body covalent interactions.

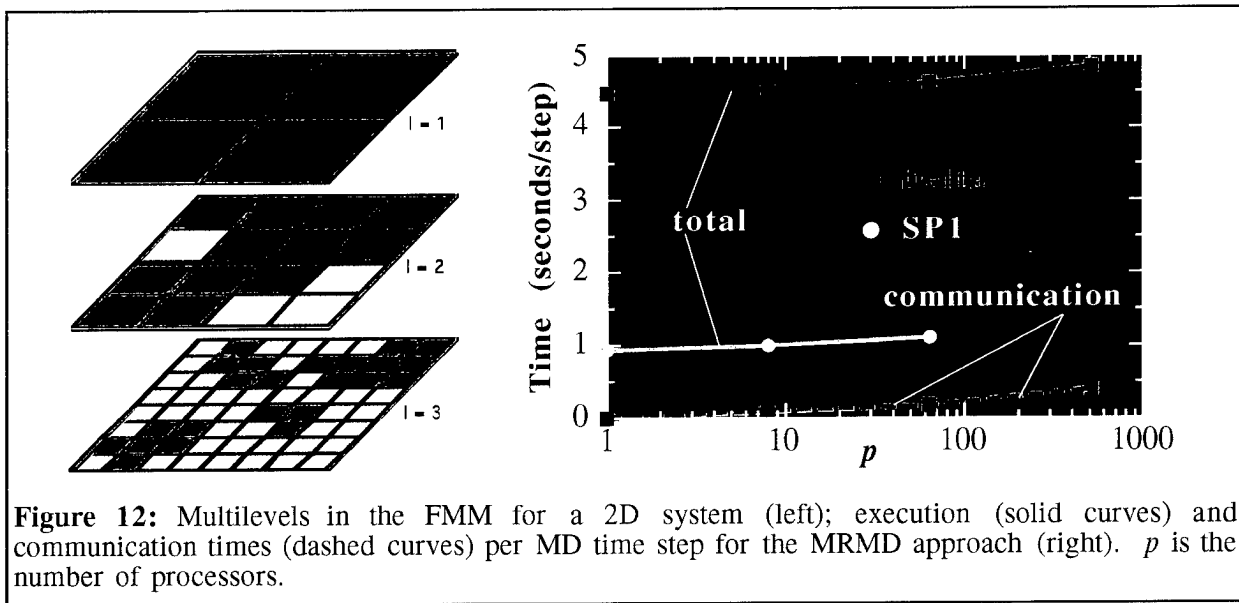


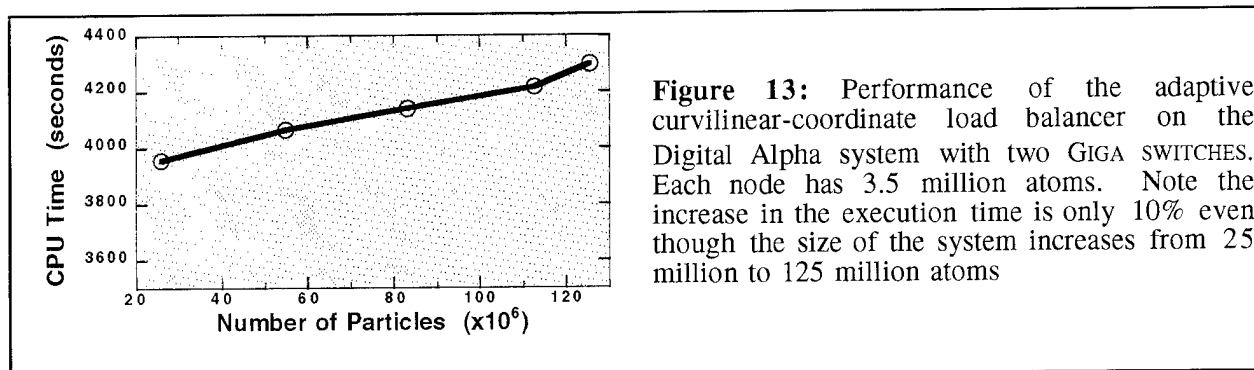
Figure 12 shows the performance of the MRMD approach on the 512-node Touchstone Delta machine at Caltech and the 128-processor IBM SP system at Argonne National Laboratory. The execution time scales linearly with the system size and the computation time dominates the communication time. Using MPI (Message Passing Interface), the MRMD has been ported to other parallel platforms as well.

§2.11 DYNAMIC LOAD-BALANCING SCHEME FOR IRREGULAR APPLICATIONS

In many atomistic simulations (e.g. porous materials or fracture) one encounters a non-uniform spatial distribution of atoms. Regular partitioning of such a system into subsystems of equal volume and then one-to-one mapping of subsystems on processors of a parallel machine leads to an imbalance of the computational workload among the processors. A load-balancing scheme has been designed by one of our students, Tim Campbell, in collaboration with Dr. Aiichiro Nakano in the Department of Computer Science. In this scheme, the computational workload is distributed equally among the processors and the interprocessor communication is minimal. In this scheme, the atomic coordinates are transformed into curvilinear coordinates:

$$\xi = \mathbf{x} + \sum_{\mathbf{Q}} a_{\mathbf{Q}} \exp(i \mathbf{Q} \cdot \mathbf{x}) . \quad (1)$$

and in the curvilinear space the system is partitioned uniformly into subsystems which are mapped onto the processors of a parallel machine. Using the simulated annealing approach, the parameters $\{a_{\mathbf{Q}}\}$ are varied so that processors have equal workloads and also the interprocessor communication is minimal. (When structural rearrangement occurs during a simulation, the variational parameters are updated dynamically to adjust the boundaries of subsystems.) Figure 13 shows the performance of this dynamic load-balancing algorithm on 36 nodes of the in-house Digital Alpha system on two GIGA SWITCHES. Evidently the algorithm performs very well even when the size of the system increases from 25 to 125 million atoms. Recently this load balancer has been further improved by replacing the plane-wave basis by orthonormal wavelets.



§ 3 INTERACTIONS/TRANSITIONS

Government Laboratories

We have a number of collaborations with scientists at government laboratories: i) We are working with Drs. Joseph Lichtenhan and Stephen Rodgers at the Phillips Laboratory; and ii) with Dr. Jeremy Broughton and his research group at the Naval Research Laboratory. We are also collaborating with a number of scientists at Argonne National Laboratory: Dr. C. Loong at the Intense Pulsed Neutron Source Division and Drs. T. Disz, W. Gropp, and R. Stevens in the Mathematics and Computer Science Division.

Industries

In collaboration with Drs. James Patterson, Joseph Manke, Daniel Curtis, Benjamin Dembart, and Thomas Wicks at Boeing Corporation, one of our students, Timothy Campbell, developed a parallel implementation of electromagnetic scattering calculations using the Fast Multipole Method (FMM).

Universities

Recently we put together an outstanding, multidisciplinary team consisting of: i) D. Brenner (North Carolina State); ii) E. Kaxiras (Harvard Univ.); iii) J. Broughton (NRL); iv) A. Madhukar (Univ. of Southern California); v) L. Greengard (Courant); and vi) T. Disz, W. Gropp, and R. Stevens (Argonne). One of our goals is to develop a materials simulation software repository which will include: i) Multiresolution schemes to carry out large-scale MD simulations based on interatomic potentials derived from electronic-structure calculations; ii) new integration algorithms that will allow MD simulations to reach microsecond time scales; iii) extensions in the areas of dynamic process support, remote memory operations, and various latency-hiding operations that will allow substantial progress in computations on heterogeneous parallel platforms; and iv) interactive and immersive visualization tools for materials simulations.

§ 4 EDUCATIONAL ACCOMPLISHMENTS: TRAINING OF GRADUATE STUDENTS

Recently we introduced an interdisciplinary program which allows graduate students to obtain a Ph.D. in physics and a M.S. from the Department of Computer Science. The aim of this program is to provide students with broad-based training in high performance computing and communications (HPCC) and the physical sciences. In connection with this program, we have introduced a number of high performance computing courses in the Physics and Computer Science Departments. The Department of Physics has two graduate courses in computational physics which are cross-listed with computer-science courses. The first course deals with classical and

quantum simulations on parallel architectures. The second course, designed for advanced graduate students, covers special topics such as multiscale phenomena, multigrid methods, wavelets, etc. In the Department of Computer Science we have introduced three new HPCC courses. Two more courses will soon be added to the computer-science curriculum: a) Heterogeneous Computing; and b) Scientific Visualization. The courses we have introduced emphasize parallel computing and algorithm design for large-scale scientific applications. Students have access to a number of parallel machines to gain hands-on experience and to perform research on large-scale computational projects.

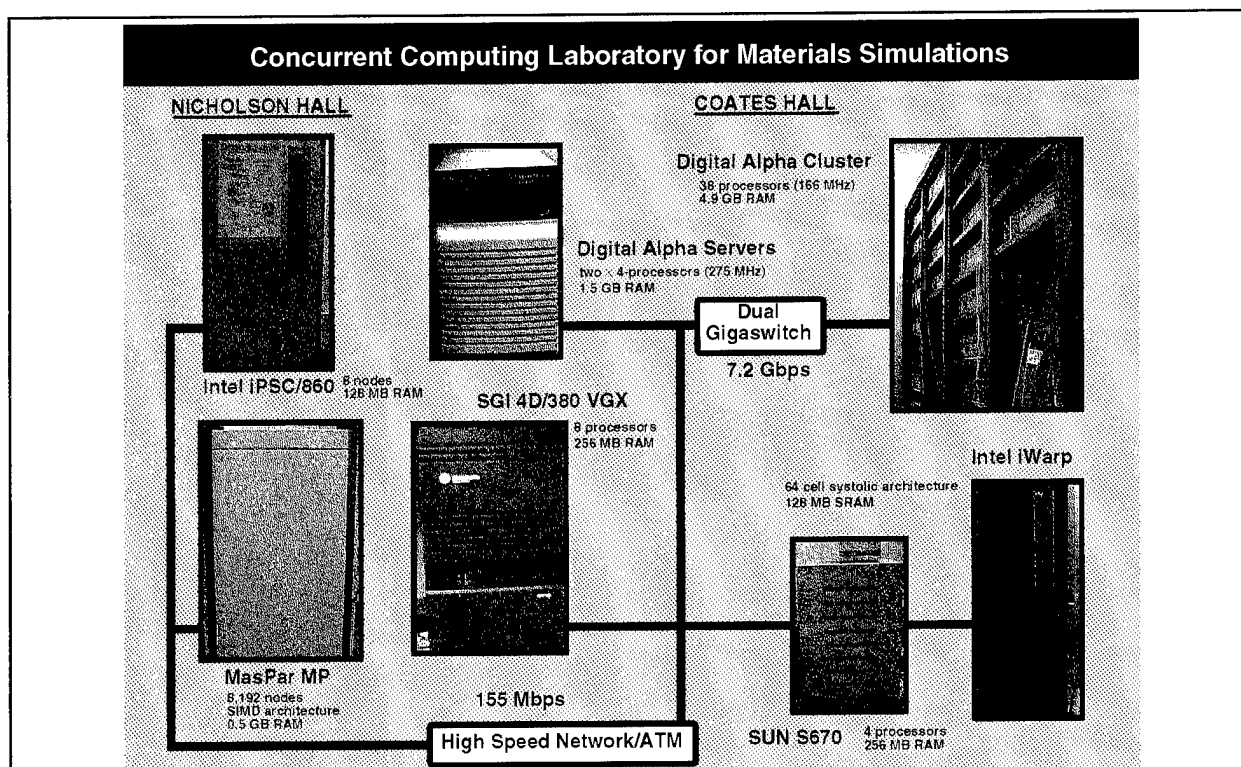


Figure 14: Computational infrastructure at our *Concurrent Computing Laboratory for Materials Simulations (CCLMS)*. The CCLMS consists of two parallel computing laboratories, one in Physics and Astronomy and the other in Computer Science. With \$2.5 million in infrastructure enhancement grants from the State of Louisiana, these labs have been equipped with the following parallel machines: **Digital Alpha cluster** - 40 Alpha nodes (46 processors consisting of eight 275-MHz and thirty-eight 165-MHz processors) connected via two Giga switches; **Intel iWarp** - a 64-cell systolic architecture; **MasPar** - an 8192-node SIMD (Single Instruction Multiple Data) machine; **Intel iPSC/860** - a distributed-memory MIMD (Multiple Instructions Multiple Data) machine. The CCLMS also has visualization facilities which include a Silicon Graphics workstation, an 8-processor Silicon Graphics Power Center, and stereo-graphic equipment. Efforts are underway to establish a virtual environment (VE) laboratory which will feature an interactive and immersive *ImmersaDesk* for visualization.

Our students also have excellent opportunities to broaden their research experience beyond the traditional university based environment. They are involved in our collaborative efforts with computational and experimental scientists at government laboratories, industries, and other universities. These interactions have significantly enhanced the research capabilities of students. Through these contacts, students also have access to excellent parallel computing and visualization facilities at other institutions.

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§ 6 INVITED TALKS

- [1] Massively Parallel Simulations of Nanostructured Materials
Texas A&M University, College Station, TX.
- [2] Multiresolution Molecular Dynamics Simulations of Real Materials Using Parallel Architectures
Livermore National Laboratory, CA.
- [3] Fracture and Sintering of Ceramic Materials by Parallel Molecular Dynamics
High Performance Computational Chemistry Workshop, Pleasanton, CA.
- [4] Large Scale Molecular Dynamics Simulation of High Temperature Ceramics
XIX International Workshop on Condensed Matter Theories, Caracas, Venezuela.
- [5] Parallel MD Simulations of Ceramic Films
Mardi Gras Conference '95, Baton Rouge, LA.
- [6] Studies of Nanoclusters and Amorphous Materials by Parallel Molecular Dynamics Simulations
Annual Meeting of the American Ceramic Society, Cincinnati, OH.
- [7] Parallel Molecular-Dynamics Simulation of Amorphous Materials
8th Annual Workshop on Recent Developments in Computer Simulation Studies in Condensed Matter Physics, Univ. of Georgia, Athens, GA.
- [8] Multimillion Atom Molecular Dynamics Experiments on Parallel Architectures
1995 Simulation Multiconference, The Society of Computer Simulation, Phoenix, AZ.
- [9] Multimillion Particle Molecular-Dynamics Simulations for Amorphous Materials on Parallel Architectures
Los Alamos National Laboratory, Los Alamos, NM.
- [10] Multimillion Particle Simulations of Real Materials on Parallel Computers
Materials Modeling '95, Naval Research Laboratory, Washington, DC.
- [11] Molecular Dynamics Simulations of Glasses and Ceramic Materials Using Parallel Computers
Takahashi Symposium, Solid State Ionics-10, Singapore.
- [12] Crack Propagation and Fracture in Ceramic Materials--Million Atom Simulations on Parallel Computers
University of Houston, Houston, TX.
- [13] Structure, Fracture and Sintering of Silicon Nitride by Parallel Molecular Dynamics
AFOSR Contractors' Conference, Washington, DC.
- [14] Dynamics and Morphology of Cracks in Silicon Nitride Films: A Molecular Dynamics Study on Parallel Computers
Materials Research Society Meeting, Fall 1995, Boston, MA.
- [15] Large Scale Molecular Dynamics Study of Amorphous Carbon and Graphite on Parallel Machines
Materials Research Society Meeting, Fall 1995, Boston, MA.

- [16] Amorphous and Liquid Carbon and Dynamic Fracture in Graphite--Molecular Dynamics Simulations on Parallel Computers
Maui Airforce Workshop, Maui, HI.
- [17] Fracture Dynamics in Crystalline and Amorphous Silicon Nitride via Parallel Molecular Dynamics
Mardi Gras Conference '96, Baton Rouge, LA.
- [18] Molecular Dynamics Simulations of Amorphous Carbon and Graphite on Parallel Machines
Mardi Gras Conference '96, Baton Rouge, LA.
- [19] Structure of Sintered Nanophase Silicon Nitride: A Molecular-Dynamics Study on Parallel Computers
Mardi Gras Conference '96, Baton Rouge, LA.
- [20] Dynamics of Fracture in Nanophase Silicon Nitride: Million Atom Molecular-Dynamics Simulations on Parallel Machines
AFOSR Meeting in Boulder, CO.
- [21] Crack Propagation and Fracture in Glasses and Ceramics--Million Atom Molecular Dynamics Simulations on Parallel Computers
Recent Progress in Computational Materials Science Symposium at the IVth International Conference on Advanced Materials, Cancun, Mexico.
- [22] Million Atom Simulations of Real Materials on Parallel Computers
SURA/EPSCoR Workshop on Computational Materials, Univ. of Kentucky, Lexington.
- [23] Million Atom Simulations of Ceramic Materials on Parallel Computers--Crack Propagation, Fracture, and Sintering in Silicon Nitride
American Ceramic Society, Indianapolis, IN.
- [24] Million Atom Molecular Dynamics Simulation on Parallel Computers
Argonne Theory Workshop, Argonne National Laboratory, Argonne, IL.
- [25] Molecular Dynamics Method and Large Scale Simulation of Amorphous Materials
NATO Advanced Study Institute on Amorphous Insulators & Semiconductors, Sozopol, Black Sea Coast, Bulgaria.
- [26] Simulation of Fracture in Silica and Carbon-Based Materials
Mardi Gras Conference '97, Baton Rouge, LA.
- [27] Mechanical Behavior of Nanophase Ceramics: Large-Scale MD Simulations on Massively Parallel Computers
Mardi Gras Conference '97, Baton Rouge, LA.
- [28] Million Atom Molecular Dynamics Simulation of Nanophase Silicon Nitride
1997 Annual Meeting of The Minerals, Metals & Materials Society, Orlando, FL
- [29] Dynamic Fracture in Nanophase Ceramics and Diamond Films: Multimillion Atom Parallel Molecular-Dynamics Simulations
International Conference on "Computer-Aided Design of High-Temperature Materials, Santa Fe, NM.
- [30] Molecular-Dynamics Simulations of Nanostructured Materials
Inelastic Nuclear Resonant Scattering Workshop, Argonne National Laboratory, Argonne, IL.